Chlorhexidine diacetate

56-95-1 | DTXSID7032345

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 6.11e-03 mol/L

Global applicability domain: Outside

Local applicability domain index: 1.66e-01

Confidence level: 3.65e-01

Nearest Neighbors from the Training Set

Image not found

Chlorhexidine
Measured: 1.58e-03
Predicted: 6.11e-03

Image not found

Guanidine, N,N'''-(iminodi-8,1-octanediyl)bis-
Measured: 2.15
Predicted: 9.84e-01

Image not found

1,3-Diphenylguanidine
Measured: 4.73e-03
Predicted: 2.00e-03

Image not found

Aziprotryne
Measured: 2.44e-04
Predicted: 1.08e-02